STRUCTURE AND INTERNAL MOTIONS OF THE PROPARGYL ALCOHOL-WATER COMPLEX

SHARON PRIYA GNANASEKAR, ELANGANNAN ARUNAN, *Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore, India*.

The rotational spectra of the propargyl alcohol (PA)–water complex has been studied using a pulsed nozzle Fourier transform microwave spectrometer. PA is multifunctional molecule having a hydroxyl group and an acetylenic moiety. We have observed a cyclic hydrogen bonded structure. The alcohol donates an H-bond to water and the acetylenic moiety accepts a weak O-H-π H-bond from water. Calculations show that the two lowest energy structures have this same structural motif and differ only in the position of the non-bonded H atom of water. Several isotopic substitutions were carried out to ascertain the position of the non-bonded hydrogen of H_2O. Rotational spectroscopy helps to differentiate between these two similar structures. Splitting of the rotational transitions was also observed, indicating the presence of internal motions of the H_2O fragment. The observed global minimum structure is compared with earlier results from IR spectroscopy in matrix[a] and helium nanodroplet[b]. We also compare the global minima of several alcohol-water complexes to understand the donor-acceptor capabilities of the OH groups in alcohol-water complexes.

[a]Saini, J.; Viswanathan, K. S. J. Mol. Struct. 2016, 1118, 147–156.

[b]Mani, D.; Pal, N.; Smialkowski, M.; Beakovic, C.; Schwaab, G.; Havenith, M. Phys. Chem. Chem. Phys. 2019, 21, 20582–20587.